Ethyl lactate 97-64-3 | DTXSID6029127

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Model	Data

Weighted KNN model

5-fold CV (7	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.84	0.55	0.85	0.53	0.83	0.64	

Model Results

Predicted value: 3.51

Global applicability domain: Inside

Local applicability domain index: 4.95e-01

Confidence level: 8.08e-01

Nearest Neighbors from the Training Set

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2,2-Dimethylpropane-1,3-diol

Measured: 4.68 Predicted: 4.44

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1,1'-Oxybis-2-propanol

Measured: 4.57 Predicted: 3.83

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3-Pyridinamine Measured: 2.09 Predicted: 3.04

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4-Aminopyridine Measured: 4.57 Predicted: 3.04

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Thiourea
Measured: 2.00
Predicted: 2.11